



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LZJ  
Title : RB69 DNA Polymerase (Y567A) ternary complex with dCTP Opposite 7,8-Dihydro-8-oxoguanine  
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Deposited on : 2010-03-01  
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

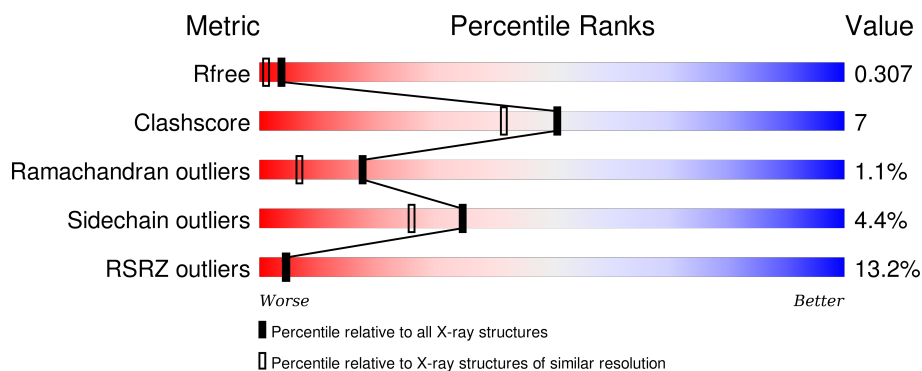
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	903	<div> <div>13%</div> <div>87%</div> <div>11%</div> </div>
2	T	18	<div> <div>11%</div> <div>56%</div> <div>28%</div> <div>17%</div> </div>
3	P	13	<div> <div>46%</div> <div>38%</div> <div>15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	8OG	T	4	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8619 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	2	0
			7385	4742	1232	1378	33			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
A	567	ALA	TYR	ENGINEERED	UNP Q38087

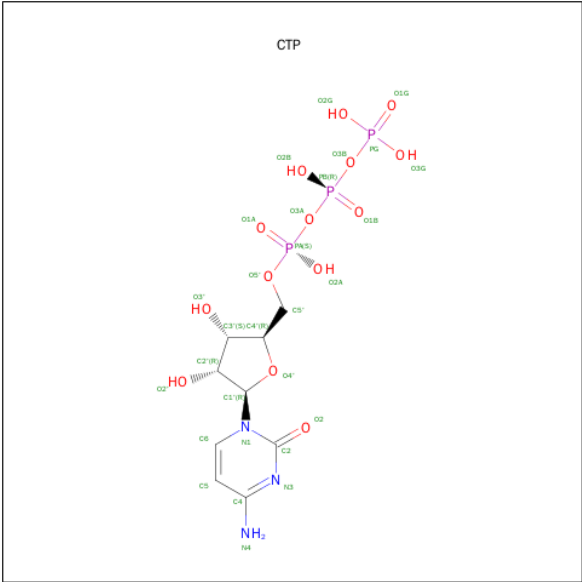
- Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*CP\*AP\*(8OG)P\*GP\*TP\*AP\*AP\*G P\*CP\*AP\*GP\*TP\*CP\*CP\*GP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	0
			372	175	71	108	18			

- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*CP\*GP\*GP\*AP\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	514	Total	O	0	0
			514	514		
6	T	38	Total	O	0	0
			38	38		
6	P	16	Total	O	0	0
			16	16		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.39Å 121.09Å 122.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.05 38.79 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.8 (38.81-2.05) 90.8 (38.79-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.205 , 0.251 0.265 , 0.307	Depositor DCC
$R_{free}$ test set	3317 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	1.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.1	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 65493 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, CA, CTP, DOC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/7569	0.57	0/10227
2	T	0.78	0/390	1.53	8/597 (1.3%)
3	P	0.77	0/273	1.41	5/420 (1.2%)
All	All	0.51	0/8232	0.71	13/11244 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	2	0

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	18	DG	O4'-C4'-C3'	-7.93	101.24	106.00
3	P	108	DC	O4'-C1'-N1	6.51	112.56	108.00
2	T	18	DG	O4'-C1'-N9	6.49	112.54	108.00
2	T	8	DA	O4'-C1'-N9	6.32	112.42	108.00
2	T	18	DG	C1'-O4'-C4'	-6.18	103.92	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	4	8OG	C4',C3'

There are no planarity outliers.



## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7385	0	7282	102	0
2	T	372	0	200	3	0
3	P	262	0	148	5	0
4	A	28	0	10	0	0
5	A	4	0	0	0	0
6	A	514	0	0	11	0
6	P	16	0	0	0	0
6	T	38	0	0	0	0
All	All	8619	0	7640	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 108 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HB3	1:A:252:VAL:HA	1.16	1.15
1:A:898:PHE:HA	1:A:899:ASP:HB3	1.29	1.15
1:A:510:VAL:HA	1:A:511:ASP:CB	1.95	0.97
1:A:251:LYS:HB3	1:A:252:VAL:CA	1.96	0.95
1:A:258:GLY:HA3	1:A:259:SER:HB2	1.46	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	903/903 (100%)	855 (95%)	38 (4%)	10 (1%)	17 7

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	259	SER
1	A	511	ASP
1	A	638	GLU
1	A	251	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	801/799 (100%)	766 (96%)	35 (4%)	35 26

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ILE
1	A	467	ARG
1	A	871	LEU
1	A	332	LEU
1	A	411	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	376	GLN
1	A	761	GLN
1	A	333	GLN
1	A	679	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	DOC	P	115	3,2	11,19,20	0.46	0	14,26,29	2.02	4 (28%)
2	8OG	T	4	2	16,25,26	2.87	4 (25%)	21,37,40	3.45	12 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DOC	P	115	3,2	-	0/3/18/19	0/2/2/2
2	8OG	T	4	2	2/2/4/4	0/3/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	4	8OG	C3'-C4'	-7.01	1.33	1.53
2	T	4	8OG	C5'-C4'	-5.76	1.33	1.51
2	T	4	8OG	O3'-C3'	-4.53	1.33	1.43
2	T	4	8OG	O6-C6	4.78	1.36	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	8OG	C2'-C1'-N9	-10.30	105.49	115.83
2	T	4	8OG	N3-C2-N1	-3.99	121.36	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	8OG	C5-C6-N1	-3.10	119.35	123.59
2	T	4	8OG	C1'-N9-C4	-2.02	124.23	127.37
3	P	115	DOC	C3'-C2'-C1'	2.20	105.16	102.71

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	4	8OG	C4'
2	T	4	8OG	C3'

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	CTP	A	904	5	21,29,30	0.85	0	33,45,47	1.54	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CTP	A	904	5	-	0/18/34/38	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	CTP	C5-C4-N3	-2.34	118.85	121.80
4	A	904	CTP	O2B-PB-O3A	3.58	121.34	105.09
4	A	904	CTP	O4'-C1'-N1	3.60	113.95	107.72
4	A	904	CTP	C2-N3-C4	4.76	122.33	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	903/903 (100%)	1.04	121 (13%) 4 4	2, 7, 27, 125	0
2	T	17/18 (94%)	0.85	2 (11%) 6 6	2, 5, 83, 105	0
3	P	12/13 (92%)	0.53	0 100 100	2, 8, 33, 38	0
All	All	932/934 (99%)	1.03	123 (13%) 4 4	2, 7, 28, 125	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	901	PHE	23.1
1	A	903	PHE	18.4
1	A	900	MET	14.6
1	A	898	PHE	13.7
1	A	897	LEU	12.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	8OG	T	4	23/24	0.96	0.19	-	2,2,4,4	0
3	DOC	P	115	18/19	0.96	0.23	-	2,2,7,8	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CA	A	905	1/1	0.94	0.22	1.16	31,31,31,31	0
5	CA	A	906	1/1	0.95	0.07	-2.59	54,54,54,54	0
4	CTP	A	904	28/29	0.98	0.08	-5.17	2,2,2,4	0
5	CA	A	908	1/1	0.89	0.10	-	59,59,59,59	0
5	CA	A	907	1/1	0.91	0.26	-	69,69,69,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.